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Extension of classical nucleation theory for uniformly sheared systems

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Abstract

Nucleation is an out-of-equilibrium process that can be strongly affected by the presence of external fields. In this paper, we report a simple extension of classical nucleation theory to systems submitted to an homogeneous shear flow. The theory involves accounting for the anisotropy of the critical nucleus formation and introduces a shear-rate-dependent effective temperature. This extended theory is used to analyze the results of extensive molecular dynamics simulations that explore a broad range of shear rates and undercoolings. At fixed temperature, a maximum in the nucleation rate is observed, when the relaxation time of the system is comparable to the inverse shear rate. In contrast to previous studies, our approach does not require a modification of the thermodynamic description, as the effect of shear is mainly embodied into a modification of the kinetic prefactor and of the temperature.

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